



## BLUE WATERS

NCSA introduces a  
new sustained-petaflop  
Cray supercomputer



## access

Vol 24 No 3 Fall 2011

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### Who we are

The University of Illinois at Urbana-Champaign's National Center for Supercomputing Applications (NCSA), one of the five original centers in the National Science Foundation's Supercomputer Centers Program, opened its doors in January 1986. Over the years NCSA has contributed significantly to the birth and growth of the worldwide cyberinfrastructure for science and engineering, operating some of the world's most powerful supercomputers and developing the software infrastructure needed to efficiently use them.

That tradition continues as the center, Illinois, Cray, and their partners in the Great Lakes Consortium for Petascale Computation develop what is expected to be the first computer dedicated to open scientific research capable of sustaining more than one petaflop, or one quadrillion calculations per second. Called Blue Waters, the system will be dedicated to massive simulations and data analysis projects that will improve our society, health, environment, and economic competitiveness. NCSA and the consortium will also work with research communities to create the new software technologies, scientific applications, and educational programs needed to take full advantage of this new system.

Blue Waters will benefit from NCSA's ongoing focus on cyberenvironments, cyber-resources, and innovative systems research. Cyberenvironments give research communities the means to fully exploit the extraordinary resources available on the internet (computing systems, data sources and stores, and tools). Cyber-resources ensure computing, data, and networking resources are available to solve the most demanding science and engineering problems and that the solutions are obtained in a timely manner. Innovative systems research involves testing and evaluating the performance of emerging computing systems for scientific and engineering applications.

NCSA also leads the Extreme Science and Engineering Discovery Environment (XSEDE), the most advanced, powerful, and robust collection of integrated advanced digital resources and services in the world. It is a single virtual system that scientists can use to interactively share computing resources, data, and expertise. Scientists and engineers around the world use these resources and services—supercomputers, collections of data, and new tools, for example—to make discoveries that benefit society. The five-year, \$121 million project is supported by the National Science Foundation. XSEDE replaces and expands on the NSF TeraGrid project. More than 10,000 scientists used the TeraGrid to complete thousands of research projects, at no cost to the scientists.

The center also leaves its mark through the development of networking, visualization, storage, data management, data mining, and collaboration software. The prime example of this influence is NCSA Mosaic, which was the first graphical web browser widely available to the general public. NCSA visualizations, meanwhile, have been a part of productions by the likes of PBS's NOVA and the Discovery Channel. Through its Private Sector Program, top researchers explore the newest hardware and software, virtual prototyping, visualization, networking, and data mining to help U.S. industries maintain a competitive edge in the global economy.

Support for NCSA is provided by the National Science Foundation, the state of Illinois, industrial partners, and other federal agencies. For more information, see

[www.ncsa.illinois.edu](http://www.ncsa.illinois.edu).

### Back cover

There is a compelling need for the development of new therapeutics that are effective against drug-resistant strains of medically important pathogens such as MRSA. A promising target is the fatty acid synthase (FAS) pathway in bacteria. Fatty acid biosynthesis is a fundamental and vital component of cellular metabolism and provides the building blocks for the formation of the bacterial cell wall. The image shows a simulation of the biocide triclosan bound to an enoyl reductase from the *M. tuberculosis* FAS pathway. Simulations are being used to optimize this lead compound for improved efficacy against drug-resistant *S. aureus*. Simulations in the lab of Carlos Simmerling, Stony Brook University.





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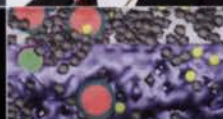
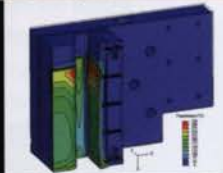
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**Thom Dunning**  
Director, NCSA



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## | An Expert Opinion |



# TRANSFORMING CO

**W**E'VE HAD SEVERAL CHALLENGING MONTHS AT NCSA, but what a comeback. Blue Waters is firmly back on track. Our new partners at Cray will begin delivering a system in the next several weeks. It will fully integrate their XE6 hardware and the next generation of their XK6 hardware. By early 2012 science and engineering researchers will be able to begin work on a 1.4 petaflops early science system (XE6), nearly doubling the computing capacity in NSF's supercomputing centers. By mid 2012, the entire Cray system will be in place.

The Blue Waters system that Cray will install in the National Petascale Computing Facility will be a CPU-GPU hybrid computing system. With its massive capability; large, fast memory subsystem; improved interconnect; and large, fast IO subsystem, it will bring sustained-petaflop performance to a broad range of science and engineering applications in fields like climate change, the spread of epidemics, earthquakes, fundamental chemistry and physics, and materials science. And, with its equally impressive GPU capability, it will serve as a bridge to the technologies on which future supercomputers will be based.

The capability and performance of the Cray system are just as relevant today as they were the first time we sat down to plan the project. Our colleagues conducting open scientific research need a system dedicated to the largest, most complex problems that can be simulated today. They'll get that with Blue Waters. Blue Waters has been configured as a balanced computing system, able to handle the most compute-, memory- and data-intensive problems in science and engineering.

It's been several months of work to bring this new plan into focus. But a few things stood out while the plan was still emerging.

They were absolutely essential to our success then and will continue to be essential as we move forward.

First among those is the NCSA staff—knowledgeable, experienced, and dedicated. All organizations do well when times are good. What distinguishes an outstanding organization is how well it does when times are uncertain. I am extremely proud of the way that our staff handled themselves during these trying times—they kept their focus on the goal and brought years of experience and expertise to bear to ensure the right outcome for the science and engineering community.

Our staff had the know-how to right the project, and they have the know-how to see that the project lives up to its fullest potential. We have everything we need to ensure that the researchers who use Blue Waters will have an outstanding computing system and technical support. With this, they will be able to take full advantage of the extraordinary capabilities that Blue Waters provides.

Cray and its impressive staff were also crucial. They entered a tricky situation with great resolve, and they've been an able partner from the outset. To say they hit the ground running is an understatement. Their commitment is obvious and greatly valued.

The entire team—at NCSA, Illinois, Cray, and our academic partners throughout the country who are part of the Great Lakes Consortium for Petascale Computation—understands the core principle behind Blue Waters. That is: It's more than just a hardware acquisition, more than just a chase for a high peak performance number or a ranking on the Top 500 list.

Instead, Blue Waters is a project that was focused from the beginning on transforming the role of computing in science and engineering. The National Petascale Computing Facility was built with flexibility in mind. The external networking for the system is



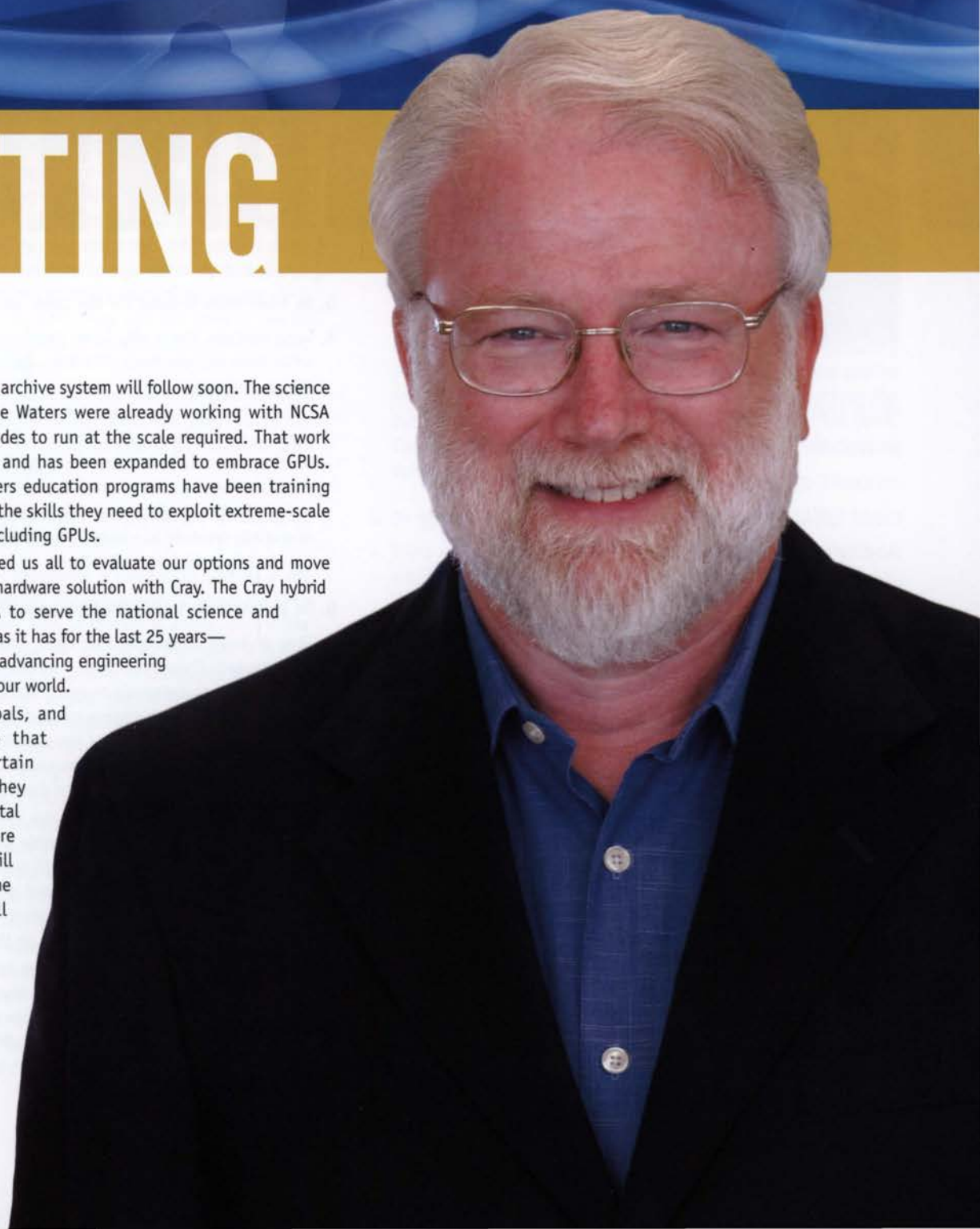
# COMPUTING

up and running, and the archive system will follow soon. The science teams who will use Blue Waters were already working with NCSA staff to prepare their codes to run at the scale required. That work is continuing unabated and has been expanded to embrace GPUs. Similarly, the Blue Waters education programs have been training hundreds of students in the skills they need to exploit extreme-scale computing systems—including GPUs.

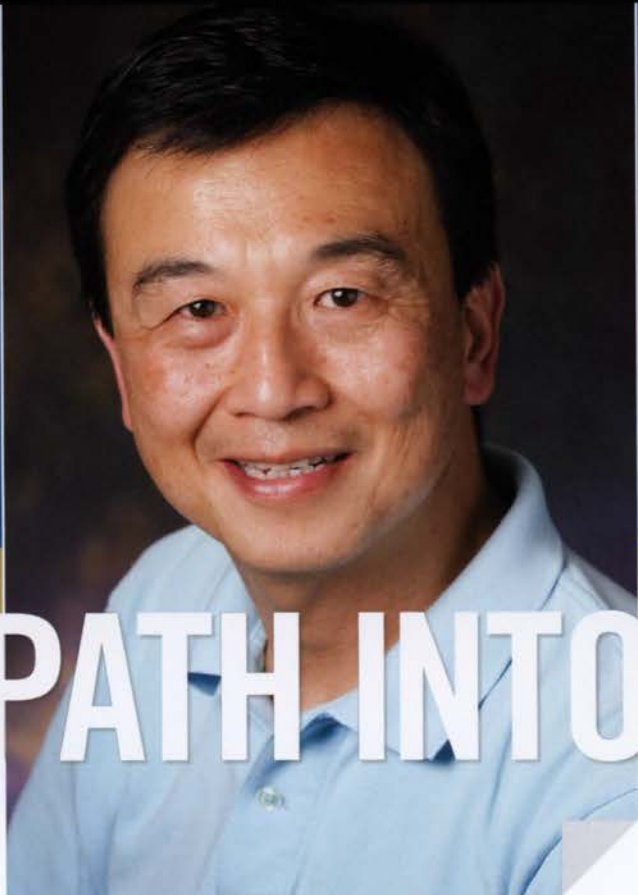
This mindset allowed us all to evaluate our options and move quickly to select a new hardware solution with Cray. The Cray hybrid system will allow NCSA to serve the national science and engineering community as it has for the last 25 years—driving new discoveries, advancing engineering practice, and improving our world.

These are lofty goals, and we are keenly aware that they come with a certain amount of risk. But they are also timeless and vital and exciting. These are the kinds of risks we will continue to take and the kind of goals we will continue to pursue.

**Thom Dunning**  
*Director, NCSA*







# PATH INTO THE FUTURE

With the announcement of a new Blue Waters petascale system that includes a substantial amount of petaflops of GPU capability, it is clear GPUs are the future of supercomputing. Access magazine's Barbara Jewett recently sat down with Wen-mei Hwu, a professor of electrical and computer engineering at the University of Illinois, a co-principal investigator on the Blue Waters project, and an expert in computer architecture, especially GPUs.

## Q. Why should we care about graphics processing units (GPUs)?

A. There are a few things about GPUs that are especially attractive. One is that if you look at a typical computer chip, a CPU chip, versus a GPU chip today, a GPU chip tends to give you 10 times more peak execution throughput and somewhere around six times of memory DRAM access bandwidth with maybe around 50 percent, in some cases only 20-30 percent, more power consumption. So if you calculate the ratios—in terms of execution throughput per watt, or memory bandwidth per watt—we're probably talking about eight times more attractive on the GPU side for the execution throughput and somewhere around five times more attractive on the memory bandwidth side.

## Q. So more work is done for the same wattage?

A. Same wattage. That's why, when people build these huge machines, GPUs have become more attractive. Because these huge machines are power hungry.

The past year was really the year where a lot of these projects turned in the GPU direction for various reasons. For two or three years we have known that those ratios are very attractive, it's just that there were other factors that deterred people from making that turn. But many of those factors have disappeared or essentially resolved to a level that this ratio started to bring people into building machines with them.

## Q. Do people have to rewrite their codes in order to run on GPUs?

A. They do have to rewrite their code. That is one of those factors I mentioned. There have been probably about five or six factors that have been deterring people from making widespread use of GPUs in the high-performance computing world. Probably the most obvious one is that the first generation of these GPUs only had single precision, the number representation used only 32 bits. Most scientific computing needs to use double precision, 64 bits.

That was a serious problem in the first—and second—generation GPUs. If you used double precision the performance dropped dramatically—more than 10 times in the first generation, and about eight times in the second generation. Go back to the performance ratio I mentioned earlier; if it drops about eight times then GPU is about the same as CPU, so there is no real advantage.

The new generation, what we call the FERMI generation, is the generation that pretty much everyone has been using since last year. The single-to double-precision performance became 1:2, exactly as a CPU now. That makes the GPU much more attractive for scientific computing.



## Questions &amp; Answers

So that's number one. Number two is it took quite a bit of time for vendors to catch up. A lot of things people use in the field were not really there for the GPUs. If you look at a lot of the scientific libraries for GPUs, the number of, say, linear algebra libraries and partial differential equation solver libraries, we have finally reached the point where it may not be all there but there are enough scientific libraries that people can begin to really use GPUs. That is why, starting last year, a lot more people were using GPUs.

Another interesting aspect is when you try to use GPUs, you can try to use them in two ways. One way is to just call the libraries; you still need to do some adjustment but it is nothing major and you avoid rewriting a lot of code. But if you want to do some form of computation that is not available in the form of libraries, you actually need to rewrite your code to run on the GPU. So this was also one of the major deficiencies.

Cray has been working on this deficiency. One of the most popular ways of programming multi-core CPUs today is OpenMP, where people write their code in C but they put in these pragmas and directives, and so on, so that the Intel compiler and some other compilers, like PTI compilers, can generate multi-threaded code for applications. With new compiler technology, people won't need to rewrite their code for GPU. They will still need to rewrite their code if they want to get a *lot* of benefit, but they won't need to rewrite to get *some* benefit.

So those are the factors that have been changing recently. If you look at the top machines in the world last year, four of the last 10 top machines were GPU clusters. That is an indication that GPUs have reached critical mass.

**Q. Will GPU codes being developed now transfer to the next generation computer? And to exascale?**

- A. GPUs need to have at least thousands of threads all running at the same time to get the full benefit of the hardware. Whereas the CPUs today typically have no more than 16 threads in a chip, even in the very high-end CPUs. When you are writing an algorithm it is very different if you are writing for 16 threads or thousands of threads. In many ways it is a redesign of your algorithm so that you can actually partition your work into much, much smaller chunks, but then all the chunks can be done in parallel. In some cases, like in solving graph problems, it is very hard.

On the other hand, if you look at exascale computing, even CPUs will have probably hundreds of threads. So we are going to cross over to the regime where you will need to be able to partition your work into smaller chunks. What is really happening is that as people begin to rewrite their code and rethink their algorithms and doing all that hard work, they make their work suitable not only for GPUs today, they are also making their code much more suitable for CPUs in the future and then definitely GPUs in the future. So that's where you are paying forward, for your future. Many application teams understand that. Essentially they are now making a one-time investment. And saying, "Once I make that investment, I make my code scaleable in terms of the number of threads. And then I have a path into the future."

One of the research projects in my lab is to actually make sure that people can truly write just one piece of code. They can just focus on getting their algorithm to be scalable. We actually have various pieces of technology to translate the code into a particular form for the GPU or a particular form for the CPU. As long as the code is based on work-efficient parallel algorithms, we have been successful in this approach. At that point, when people invest in developing their new code, they are not just investing into GPU only, they are investing into the future path.

**Q. Gets them thinking of the big picture?**

- A. Another important activity is that we're teaching a lot of these chip-level scalable programming techniques to domain people, people in physics, mechanical engineering, and so on. It's not that we expect everyone to be writing detailed code, but we're actually training them to *think* about scalable programming, so they can begin to also renew their models, their methods. Begin to think about parallelism and data locality in a competent way. They can work with people who are really good with libraries and coding and so on to be able to develop a new generation of libraries faster.

We recognized this need for education and planned for it when we wrote the Blue Waters project proposal. That is why there is the Virtual School of Computational Science and Engineering (VSCSE) summer school; we already knew these things were coming and made it part of the project. I have also been teaching the European Union summer school in Barcelona for the past two years. These schools are really about training the domain scientists to think about scalable computation.

**Q. So GPUs have arrived. Are people willingly converted?**

- A. There are a couple of things that are interesting. In some of these application domains, such as in molecular dynamics, for example, if you look at the entire application—not just the part you move to the GPU, but after you move these parts to the GPU—if you look at the entire application often times we are talking about two times speedup, in some cases three to four times speedup versus the 10 times peak execution throughput I previously mentioned. In some cases people have demonstrated for some routines you can actually get close to 100 times speedup because of the interaction between the memory bandwidth and the peak performance. But usually that is less common. So people will say, what's the big deal? For the whole application, you are only getting two or three times speedup. But I think it is something we need to put into perspective.

We are at the point in the industry where just the computing power grows about two times every two years. But in terms of real application, often you are getting less than 40 percent. Again, the growth is two times in terms of *peak* performance, but not in terms of real application. People don't realize this. They think, "I'll just wait another two years and I'll get two times." I have to tell them no, you don't understand. In another two years you'll be getting probably 40 percent performance increase and you still have to work for it.



## Questions &amp; Answers

So in order to actually get two times in terms of real application performance increase, in terms of this natural evolution, you will have to get around six times increase in terms of the peak. And guess what? That's going to be *eight years* from now. And that becomes an extremely obvious situation. If it is going to be eight years, it is much better if you can get some increase today.

**Q. Is that some of the problem the HPC industry has had—we get so focused on the Top500 list and peak performance?**

A. Yes. The whole HPC industry is going toward lower clock frequency and higher throughput types of systems. That is why most people are exploring GPUs for their computations. When you think about development efforts and when you think about sustained performance, real application performance, this is different than what we talk about in terms of peak.

For the new Blue Waters design, the GPU nodes are going to be very, very strong nodes. So as long as we can develop good node-level algorithms, these nodes are going to be even stronger than the old Blue Waters design. To me, that is extremely important because that means if we do a good job getting the node level algorithms, then we can actually sustain a higher level percent of performance for the applications. But you know, these are the challenges that we still need to meet. These are real challenges.

**Q. Take it from scientific computing into personal computing. Are we going to be having GPUs on our desks and in our laptops?**

A. Oh, absolutely. Every computer has a GPU in it, that's the graphics card. At this point, not all those graphics cards are what we call CUDA-enabled, or GPU-computing-enabled, but at this point every graphics card shipped by NVIDIA is pretty much GPU-computing-enabled. So in a few years, everything that you can buy, and pretty much everything that people use, will be GPU-computing-enabled.

That's actually extremely important, because when people take the time and effort to write their code in a form that can execute well on GPUs, they want to be able to run them on millions and millions of systems. We've had these exotic parallel machines and have maybe 100 of them in the world. People just ignore them because there is no real money in selling software or licensing software for those machines. With only 100, how many customers can there be?

But here you have hundreds of millions of machines. That's the fundamental reason why people are willing to port all the libraries, because those libraries cost a lot of effort and money. Since all these machines will have GPU-computing capabilities, those libraries can now run on hundreds of millions of machines instead of just being used by HPC people. So now there is a business case for that.

Another important consideration is, if you look at the mobile world there is now a design style called fusion that essentially has a single chip with a modest CPU and a modest GPU on it. These chips are very power efficient, but they have a fair amount of computing power from the GPU. We're talking probably 100 gigaflops. Compared to the high-end GPU that is about 2 teraflops today, 100 gigaflops is not a whole lot, but if you compare

that with the high-end CPUs today, most CPUs are still at about 60 gigaflops. So these chips you can put into tablets and the like will have 100 gigaflops, and that gives you tremendous computing power with very low energy consumption for very sophisticated applications. Even on cell phones in the future.

That actually brings out some very interesting client applications. Suddenly the smartphones don't need to necessarily rely on all servers for executing applications, they can have much, much better use of interfaces and they can have much better latency. Because for some of these applications, if you want to talk with them in a server, the latency of communication to a server incurs intolerable latency. So now we're beginning to see even more interest in developing applications and libraries for GPUs for that reason.

**Q. With solving some of these issues with GPUs, does that, in your opinion, make exascale something we are now going to be able to hit?**

A. No! It is still not clear to me if we can hit exascale. Even with GPUs we're still not quite there yet. We're still probably another order of magnitude short. If you look at the GPU floating-point performance per memory, per gigabyte of main memory, it is still not quite sufficient. In the future we're going to have dramatically less amount of memory available per gigaflop of performance. That will further require some even worse brain surgery for many, if not most, of the algorithms. When I look at some of these things, it is still not clear to me how some of those problems will be solved. So much of that is still going to be research.

**Q. So we still have things to dream about.**

A. Yes. And there are still going to be a lot of inventions. And that's also the scary part. People still need to invent new algorithms and people still need to invent probably some of these new models to be able to fill that one order of magnitude gap that nobody really knows how to fill at this point.

**Q. Do you think funding constraints will hinder innovation, or will it encourage even more creativity?**

A. That's hard to tell. Funding has always been kind of funny. In reality, nobody really funds these things. If you look at the way the National Science Foundation and the Department of Energy spend money on these machines, they are always quick in spending money on the hardware. But they are always reluctant to spend money on the applications and the software. Moving forward, I think it is going to be the same. But people always manage to put together some money for these innovations. So I think it may still happen. But there is going to be a lot of uncertainty, and I think it may come more slowly than people imagine.



# PRAC TEAMS COVER MANY DISCIPLINES

**W**ITH THE BLUE WATERS SUSTAINED-PETASCALE COMPUTER, researchers will be able to gain important insights into problems some have been exploring for years. To take full advantage of the new technologies of Blue Waters, however, codes must be improved. Petascale Computing Resource Allocations (PRAC awards) from the National Science Foundation allow research teams to work closely with the Blue Waters project team in preparing their codes. The codes and projects address key challenges faced by our society and explore fundamental scientific and engineering problems.

The collaborations with the Blue Waters team include help porting and re-engineering existing applications. In some cases, the teams will build entirely new applications based on new programming models.

Current projects represent a wide range of disciplines. They will drive scientific discovery for years to come. Projects are:

**Accelerating nano-scale transistor innovation—Principal Investigators:** Gerhard Klimeck, Thomas Hacker, Purdue; Mathieu Luisier, Purdue University

**Simulating vesicle fusion on Blue Waters—Principal Investigators:** Vijay Pande, Stanford University

**Using petascale computing capabilities to address climate change uncertainties—Principal Investigators:** Donald Wuebbles and Xin-Zhong Liang, University of Illinois at Urbana-Champaign

**Hierarchical molecular dynamics sampling for assessing pathways and free energies of RNA catalysis, ligand binding, and conformational change—Principal Investigators:** Thomas Cheatham, University of Utah; Darrin York, Rutgers University; Carlos Simmerling, State University of New York at Stony Brook; Adrian Roitberg, University of Florida; Ross Walker, San Diego Supercomputer Center

**Petascale multiscale simulations of biomolecular systems—Principal Investigators:** Gregory Voth and Benoit Roux, University of Chicago

**Petascale plasma physics simulations using PIC codes—Principal Investigator:** Warren Mori, University of California-Los Angeles

**Type Ia supernovae—Principal Investigators:** Stanford Woosley, University of California Observatories; Michael Zingale, State University of New York at Stony Brook; John Bell, Lawrence Berkeley National Laboratory

**Enabling breakthrough kinetic simulations of the magnetosphere via petascale computing—Principal investigators:** Homayoun Karimabadi, Kevin Quest, Amitava Majumdar, University of California-San Diego

**Super instruction architecture for petascale computing—Principal Investigator:** Rodney Bartlett, University of Florida

**Simulation of contagion on very large social networks with Blue Waters—Principal Investigators:** Keith Bisset, Virginia Tech; Shawn Brown, Carnegie-Mellon University; Douglas Roberts, Research Triangle Institute

**Computational relativity and gravitation at petascale: Simulating and visualizing astrophysically realistic compact binaries—Principal Investigator:** Manuela Campanelli, Rochester Institute of Technology

**Electronic properties of strongly correlated systems using petascale computing—Principal Investigators:** Kristjan Haule, Rutgers University New Brunswick; Sergey Savrasov, University of California-Davis

**Petascale research in earthquake system science on Blue Waters—Principal Investigator:** Thomas Jordan, University of Southern California

**Testing hypotheses about climate prediction at unprecedented resolutions on the NSF Blue Waters system—Principal Investigators:** Benjamin Kirtman, University of Miami; William Large, University Corporation for Atmospheric Research; David Randall, Colorado State University; Cristiana Stan, Institute of Global Environment and Society

**Computational chemistry at the petascale—Principal Investigator:** Monica Lamm, Iowa State University

**Peta-Cosmology: galaxy formation and virtual astronomy—Principal Investigator:** Kentaro Nagamine, University of Nevada, Las Vegas

**Formation of the first galaxies: predictions for the next generation of observatories—Principal Investigator:** Brian O'Shea, Michigan State University

**Enabling science at the petascale: From binary systems and stellar core collapse to gamma-ray bursts—Principal Investigator:** Erik Schnetter, Louisiana State University & Agricultural and Mechanical College

**The computational microscope—Principal Investigator:** Klaus Schulten, University of Illinois at Urbana-Champaign

**Lattice quantum chromodynamics on Blue Waters—Principal Investigator:** Robert Sugar, University of California, Santa Barbara

**Petascale simulations of complex biological behavior in fluctuating environments—Principal Investigator:** Ilias Tagkopoulos, University of California-Davis

**Enabling large-scale, high-resolution, and real-time earthquake simulations on petascale parallel computers—Principal Investigator:** Liqiang Wang, University of Wyoming

**Understanding tornadoes and their parent supercells through ultra-high resolution simulation/analysis—Principal Investigator:** Robert Wilhelmson, University of Illinois at Urbana-Champaign

**Petascale simulation of turbulent stellar hydrodynamics—Principal Investigator:** Paul Woodward, University of Minnesota-Twin Cities

**Petascale computations for complex turbulent flows—Principal Investigator:** Pui-Kuen Yeung, Georgia Institute of Technology

**Breakthrough petascale quantum Monte Carlo calculations—Principal Investigator:** Shiwei Zhang, College of William and Mary □





# CATCH THE WAVE





by Barbara Jewett

## Modeling and simulation using NCSA resources

help scientists advance work

with supernovas.

O

**VERHEAR** Robert Fisher and Gaurav Khanna discussing hotel stars and catching the wave, and you'd think they're discussing a recent vacation. Wait. Now the conversation has shifted to Type Ia. Isn't that the person who thrives on work?

The University of Massachusetts Dartmouth professors are really talking about their collaboration on groundbreaking computational astrophysics research—their team is the first to successfully predict the gravitational wave signature for Type Ia supernovae. These researchers believe that scientists should explain their work in a manner such that others can learn from them and understand the importance of what they do. Often this requires using analogies easy for non-scientists to grasp.

Exploding stars, or supernovae, “are just intrinsically wonderful and interesting systems to study,” says Fisher. Type Ia supernovae are the result of explosions of white dwarf stars.

“A white dwarf is like a retirement for stars,” says Fisher. “They’ve had their careers burning nuclear fuels and they go off to the retirement home or retirement hotel, continuing to sort of shine although they are no longer working, no longer burning nuclear fuels. They just are living off their retirement account if you will, giving off whatever remnant heat they have in the form of visible light.”

After billions of years of active nuclear burning, the white dwarf heads off to the retirement hotel with its companion, a binary star. And that binary star can donate mass to the white dwarf through a process called accretion, Fisher explains. But the donation can drive the white dwarf to the point of instability and it explodes, becoming a supernova.

The team’s groundbreaking research also demonstrated what researchers can do with modern supercomputers. Fisher has used high-performance computers at NCSA since 1992, when he was a sophomore in college and worked with Ronald Taam at Northwestern doing computational astrophysics.

“I go way back, almost to the very beginning of NCSA,” he says with a laugh. “And note, I’m not that old! I can see from my research, and from the students I’ve trained to use supercomputers, they’ve just had such a huge impact. It is impossible to estimate what the true value is. It is truly an amazing resource, to have a national center for supercomputing.”

Only in the last few years, however, have the sizeable advances in computing power made it possible to study the evolution of a supernova from first principles simulations in three dimensions. “These models are so extremely realistic, it’s incredible,” he says.

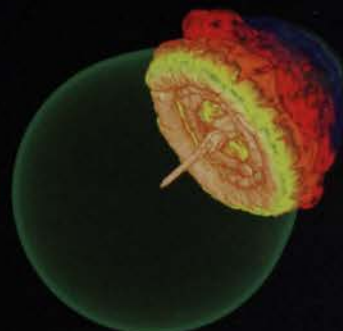
Master’s student David Falta assisted the project, running 3D simulations on NCSA’s now-retired Abe cluster in addition to the



Images : Flash Center, University of Chicago



(a) The simulation is initiated near the endpoint of the white dwarf's lifespan, when a single nuclear flame bubble has been ignited near its center. The buoyancy of the bubble rapidly pushes it up to the surface of the white dwarf.



(b) Within one second of physical time, the bubble emerges from the surface of the white dwarf.

Louisiana Optical Network Initiative's QueenBee. The team's results were published earlier this year in *Physical Review Letters*.

### Gravitational waves

Currently, researchers are only able to study the Type Ia supernovae in visible light, which comes out over weeks and months. This is due to the fact that even though the real-time white dwarf explosion into a Type Ia supernova only lasts about two seconds, the star shrouds the information that initially comes out in the visible light, making it nearly opaque.

Gravitational waves, on the other hand, go through anything very freely. That's what makes them so hard to detect but also what makes them amazing sources of information, says Fisher. The actual process of the two-second explosion would be "right there in the gravitational wave."

The team looked at the simulated explosions with a fresh viewpoint. Instead of just trying to simulate the supernova explosion, they explored the consequences of it.

By focusing on the consequences, they noticed the explosion doesn't originate from the star's center; the explosion is asymmetric. Recent optical measurements by Keiichi Maeda of the University of Tokyo and colleagues, published in *Nature*, have independently confirmed that Type Ia supernovae are asymmetric.

Albert Einstein's Theory of Relativity predicts that if you take a large amount of mass that is asymmetric, it will give off another form of radiation that is not seen by visible light but is actually a distortion in space and time, explains Khanna.

"If you have violent events that are very asymmetric, like a Type Ia supernova, that can cause a ripple in spacetime that travels at the speed of light," he says. "So, very much like if you were to throw a pebble on the surface of a pond that causes ripples, you would have a ripple propagating outward. But this would be a ripple in spacetime itself.

And this ripple would be what we call gravitational waves, and would eventually come to us on Earth and we would be able to detect them."

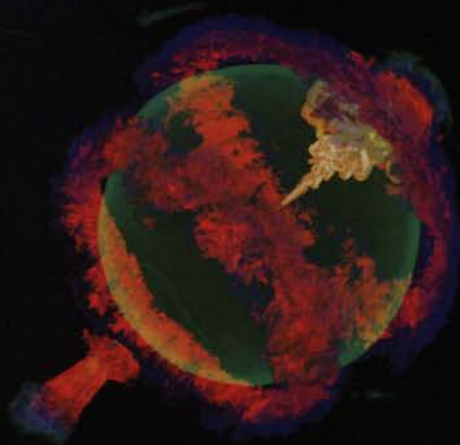
The ability of gravitational waves to pass through matter without corruption of information, or any kind of issue, "and get to us, carrying that information," is one of the reasons behind the emerging field of gravitational wave astronomy, notes Khanna. Using gravitational waves supplements what astronomers learn from light.

"And if we can read that information, using gravitational wave detectors, we would have high-quality information about any source we're studying," he says.

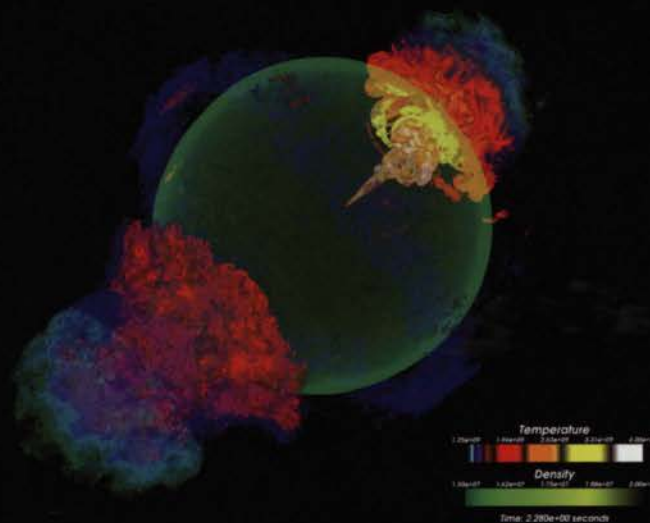
Direct detection of cosmic gravitational waves has long been sought. The Laser Interferometer Gravitational-Wave Observatory, or LIGO, is a large-scale physics experiment to detect gravitational waves and develop gravitational-wave observations as an astronomical tool. Funded by the National Science Foundation, the project is operated by Caltech and the Massachusetts Institute of Technology. Research is carried out by the LIGO Scientific Collaboration, a group of more than 800 scientists at universities around the United States and in 11 foreign countries. The project has observatories in Hanford, Washington, and Livingston, Louisiana.

But all gravitational waves are not equal. Drawing again on a non-science comparison, Fisher explains that if you could tap a white dwarf star it would ring like a bell, tinkling about every second because of its relatively high density—over a billion times that of water at its center. Compare that to our sun, he says, which would oscillate slowly and ring about once every 30 minutes if tapped. That characteristic ringing frequency is usually about the characteristic frequency of the gravitational wave emission. Extremely dense astrophysical sources, such as neutron stars and black holes, ring at very high frequencies, up to a thousand times a second—right in the range of LIGO. Because Type Ia supernovae are less dense than neutron stars and black holes,





c) The ash rushes over the surface of the white dwarf, which remains intact and gravitationally-bound, culminating in an intense jet which sets off a detonation on the opposite end of the star about one second later.



(d) The resulting detonation releases an amount of energy comparable to the entire luminous output of our sun in a fraction of a second.

their gravitational waves are at a lower frequency than these events, about 1 Hertz, he says.

### Catching the wave

Khanna emphasizes that Type Ia gravitational waves are not detectable with current instruments. While LIGO may have advanced instruments detecting neutron stars and white dwarfs in 2014 or 2015, he says, LISA, the Laser Interferometer Space Antenna, would be more likely to capture the Type Ia's lower frequency gravitational waves. This is because instead of being ground-based, it will actually be an antenna orbiting in space.

LISA was to be a joint project of NASA and the European Space Agency (ESA). Due to budget cuts, NASA pulled out of the project early in 2011. ESA is planning to continue the project, but it most likely will be at a smaller scale, which may then limit the antenna's ability to capture the Type Ia waves. Future planned spaceborne instruments, including the Big-Bang Observer, currently under consideration by NASA, are more ideally suited to the detection of Type Ia supernovae.

But until then, the team's work is a starting point.

"We were able to show Type Ia's have a gravitational wave signature, and make a prediction of what the gravitational wave signature would be. That was a first that came out of this work," says Fisher.

"When we first did this study, we thought the chance of a supernova exploding close enough to be easily detectable by future instruments would be quite serendipitous. Then just as the ink on our paper was drying, astronomers caught the closest Type Ia in half a century, SN 2011fe. This supernova would have been detected in gravitational waves by the proposed Big Bang Observer mission," he added.

In the meantime, modeling and simulation will have to suffice. Hopefully, one day in the next decade, another supernova like SN

2011fe will once again light the skies, finally allowing Robert Fisher and Gaurav Khanna to catch the wave. □

## PROJECT AT A GLANCE

### TEAM MEMBERS

David Falta  
Robert Fisher  
Gaurav Khanna

### FUNDING

National Science Foundation

### FOR MORE INFORMATION:

[www.novastella.org](http://www.novastella.org)  
[www.ligo.org](http://www.ligo.org)  
<http://lisa.nasa.gov/>  
<http://flash.uchicago.edu/site/movies/GCD.html>

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# NCSA, CRAY PARTNER ON BLUE WATERS SUPERCOM

**T**HE UNIVERSITY OF ILLINOIS' National Center for Supercomputing Applications (NCSA) has finalized a contract with Cray Inc. (Nasdaq: CRAY), to provide the supercomputer for the National Science Foundation's Blue Waters project.

This new Cray supercomputer will support significant research advances in a broad range of science and engineering domains, meeting the needs of the most compute-intensive, memory-intensive, and data-intensive applications. Blue Waters is expected to deliver sustained performance, on average, of more than one petaflop on a set of benchmark codes that represent those applications and domains.

More than 25 teams, from a dozen research fields, are preparing to achieve breakthroughs by using Blue Waters to model diverse phenomena, including: nanotechnology's minute molecular assemblies, the evolution of the universe since the Big Bang, the damage caused by earthquakes and the formation of tornadoes, the mechanism by which viruses enter cells, and climate change.

Blue Waters will be composed of more than 235 Cray XE6 cabinets based on the recently announced AMD Opteron™ 6200 Series processor (formerly code-named "Interlagos") and more than 30 cabinets of a future version of the recently announced Cray XK6 supercomputer with NVIDIA® Tesla™ GPU computing capability incorporated into a single, powerful hybrid supercomputer. These Cray XK nodes will further increase the measured sustained performance on real science problems.

"We are extremely pleased to have forged a strong partnership with Cray. This configuration will be the most balanced, powerful, and useable system available when it comes online. By incorporating a future version of the XK6 system, Blue Waters will also provide a bridge to the future of scientific computing," said NCSA Director Thom Dunning.

"The project is an incredible undertaking, requiring commitment and dedication not only from NSF, NCSA, the University of Illinois, and the science teams, but also from our computing systems partner—Cray. This strong partnership further establishes our place at the

forefront high-performance computing," said University of Illinois President Michael Hogan.

"The Blue Waters team has the technological capability and the commitment to make this important resource a reality—a resource that will help scientists and engineers solve their most challenging problems," said Phyllis Wise, chancellor of the University of Illinois at Urbana-Champaign.

#### The Cray Blue Waters system will employ:

- Cray's scalable Gemini high-performance interconnect, providing a major improvement in message throughput and latency.
- 8-core AMD Opteron™ 6200 Series processors, selected by the editors of HPCwire as one of the top five new technologies to watch in 2011.
- Cray XK6 blades with NVIDIA® Tesla™ GPUs, based on NVIDIA next-generation 'Kepler' architecture, which is expected to more than double the performance of the Fermi GPU on double-precision arithmetic.
- 1.5 petabytes of total memory (or four gigabytes per AMD Opteron 6200 Series processor core).
- Cray's scalable Linux Environment (CLE) and HPC-focused GPU/CPU Programming Environment (CPE).
- A Cray integrated Lustre parallel file system with more than one terabyte-per-second of aggregate storage bandwidth and more than 25 petabytes of user accessible storage.
- Up to 500 petabytes of near-line storage and up to 300 gigabits per second of wide area connections.

"We are extremely proud to have been selected to deliver the Blue Waters system through this important partnership with the NSF, the University of Illinois, and NCSA," said Peter Ungaro, president and CEO of Cray. "It's a honor to be able provide the NSF's vast user community with a Cray supercomputer specifically designed for delivering real, sustained



# SUSTAINED-PETASCALE COMPUTER

petascale performance across a broad range of breakthrough science and engineering applications. It's a passion that drives all the members of this partnership, and we are pleased to be a part of it."

Consisting of products and services, the multi-year and multi-phase contract is valued at more than \$188 million. Cray will begin installing hardware in the University of Illinois' National Petascale Computing Facility soon, with an early science system expected to be available in early 2012. Blue Waters is expected to be fully deployed by the end of 2012.

As supercomputers continue to grow in scale and complexity, it becomes more challenging to effectively harness their power. Since the Blue Waters project was launched in 2008, NCSA has helped researchers prepare their codes for the massive scale of this and other extreme-scale systems. NCSA also initiated a broad range of R&D projects designed to improve the performance of the existing HPC software stack and facilitate the development and use of applications on Blue Waters and other petascale computers.

The Blue Waters project is now prepared to mount a major, community-based effort to move the state of computational science into the petascale era. The center will work with the computational and computer science and engineering communities to help them take full advantage of Blue Waters as well as future supercomputers. The effort will focus on scalability and resilience of algorithms and applications, the use of accelerators to improve time to solution for science and engineering problems, and enabling applications to simultaneously use computational components with different characteristics. □

For more information about the Blue Waters project, see:  
<http://www.ncsa.illinois.edu/BlueWaters/>.

## BLUE WATERS STATS

Cray XE6 cabinets:	>235
Cray XK6 cabinets:	>30
Total cabinets, including storage & server cabinets:	>300
Compute nodes:	>25,000
Usable Storage Bandwidth:	>1 TB/s
Aggregate System Memory:	>1.5 Petabytes
Memory per core:	4 GB
Interconnect Topology:	3D Torus
Number of disks:	>17,000
Number of memory DIMMs:	>190,000
Usable storage:	>25 Petabytes
Peak performance:	>11.5 Petaflops
Number of AMD processors:	>49,000
Number of AMD x86 cores:	>380,000
Number of NVIDIA GPUs:	>3,000
External network bandwidth:	100 Gb/s scaling to 300 Gb/s
Integrated near line environment:	scaling to 500 PBs
Bandwidth to near-line storage:	100 GB/s



BEHIND THE SCENES OF NCSA

BLUE W







**TO CREATE AN INCREDIBLE RESOURCE** like the Blue Waters supercomputer takes an incredible team. In addition to the project's principal and co-principal investigators, project managers, and hardware and software architects, dozens of NCSA staffers work behind the scenes, moving the project forward.

Programmers writing code. Accounting analysts tracking expenditures. Assistants keeping the meetings organized. Audio-visual technicians ensuring transmission clarity in video meetings and conference calls. Educators developing course curriculum. Webmasters sharing the team's work with the world. Research scientists applying the analytical skills and innovation that NCSA is known for.

Every day, over 60 people at the center use their technical knowledge and expertise to deal with the thousands of minute details involved in a project of this magnitude. Their eyes are on the ultimate goal: providing an incredible computing resource for the nation's scientists and engineers in 2012. ▣

# WATERS



By Allison Copenbarger  
& Barbara Jewett

# FROM ALLIANT

**F**OR MANY PEOPLE, a first summer job may be a memory best forgotten. But Brian Thomas' first job at a steel company proved to be both memorable and life altering.

When Thomas was a 20-year-old undergraduate student majoring in engineering, he worked at a large Canadian steel producer and became fascinated by the process of continuous casting steel—the process that turns molten steel into sheets and that is used to produce 92 percent of the world's steel. He decided he would like to use his engineering skills to refine the process.

Thomas went on to earn a PhD in metallurgical process engineering at the University of British Columbia and took a position on the mechanical engineering faculty at the University of Illinois. Now, 26 years later, Thomas' research is regarded as some of the top in his field and he is the director of the Continuous Casting Consortium (CCC), a cooperative research effort between his research group at the university and the steel industry.

With annual global steel production at almost 1.5 billion tons (100 million tons in the United States, 96 percent of that through continuous casting), steel production accounts for an important fraction of the total energy consumed and greenhouse gases produced in the world. Even small improvements to this process, says Thomas, can have a profound benefit to society.

"For me the idea is to take this process which looks to outsiders kind of Dark Ages—crude and as empirical as you can get—and combine that with high technology," he says.

## HPC changes an entire industry

High technology is where NCSA comes in. Thomas began his career at Illinois around the time NCSA opened its doors, so his research has been linked to the center since its beginning. "We've sort of grown up together," he says, noting he's used every computer from Alliant (and Cray X-MP) to the new Forge.

And the center has provided Thomas more than just compute cycles. NCSA research scientist Seid Koric has worked closely with Thomas for over 10 years to develop better algorithms for modeling

thermal stress in steel continuous casting. After joining NCSA, Koric began work on an engineering PhD and became a member of Thomas' research group; the two have collaborated ever since. This unique research relationship with an NCSA collaborator has produced many important tools and findings.

Many steel processes, such as continuous casting, involve multiple coupled phenomena, including fluid flow, heat transfer, solidification, distortion, and stress generation. The computational complexity of the phenomena is so high that it challenges the capabilities of even the best numerical methods and computer hardware. Consequently, there is a growing need to use high-performance computing resources and better algorithms to make these simulations feasible. To enable realistic quantitative predictions of the formation of defects in these commercial solidification processes, high-fidelity simulations are needed, and with today's compute resources they are now starting to become possible, says Thomas.

Koric and Thomas have developed several ground-breaking numerical methods for solving highly nonlinear, complex multiphysics problems that they've applied to their simulations to gain new insights into the continuous casting process. For instance, an algorithm for constitutive-equation integration was implemented into the commercial finite-element code Abaqus, which improved the code's performance in solving solidification stress problems on HPC machines by more than an order of magnitude. For the first time, it demonstrated and verified the significant advantages in scale-up for large three-dimensional problems on parallel computers.

And a new enhanced latent heat method was recently developed by Koric.

## The steel-making process

Though the process of making steel "has been around for millennia," says Thomas, it is very intricate and complicated to continuously cast steel into sheets.

The steel is first produced in batches and delivered in ladles. The steel flows from the ladle into the tundish via a nozzle to protect the metal from oxidizing in the air. The tundish, a pouring box that holds



# TO FORGE

NCSA supercomputers support years of steel research.

the molten steel and then continuously delivers it to the mold, serves to remove most of the harmful inclusions.

In the mold, the molten steel freezes against water-cooled copper walls. The mold oscillates vertically to prevent sticking. The machine also withdraws the solidified metal from the mold through the bottom at the same rate that the molten metal flows into the mold—sensors control this perfect rate.

After leaving the mold, the metal is solid only on the outside. It is transported between support rolls and sprayed with water until the center is completely cooled. Then the steel is cut to the desired size.

Thomas explains that a slight change in any of these stages could create vast differences and defects in the final product. For example, changing the geometry of one nozzle can make a defect appear or disappear.

Or if the fluid flow and solidification are not perfectly set, there can be a “breakout,” in which molten steel pours through a crack in the partly-solidified casting, covering the area with superheated molten steel, which is very dangerous for the workers and costly for the steel plant.

## Computer modeling aids industry

Thomas and his team have modeled all aspects of the continuous casting process: turbulent fluid flow, transfer by nozzles, heat transfer, stresses and strains, and solidification. According to Thomas, one important success has been the pioneering work of understanding the mixing of different steel grades.

Higher-quality grades of steel are very expensive, so contaminating them with a different grade would produce a costly, low-quality product. But stopping and restarting the process is also costly. Thus, casting different grades together in sequences benefits from the predictions of computational models of the mixing. Steel production is a high-volume, low-profit-margin industry. Improved efficiency

and consistent steel quality, relative to low-cost alternatives, means producers realize more profit. Better understanding of how defects form, explains Thomas, allows steel continuous casters to produce steel with fewer defects and operate at a higher casting speed, which in turn enables higher production rates (and accompanying efficiencies), and also yields better energy efficiency, such as less furnace time needed after casting to reheat the slab back up to rolling temperatures.

“What most people don’t realize,” says Koric, “is that Brian Thomas is THE go-to guru for the steel industry. Everybody in the world comes to Brian and the University of Illinois to solve their problems, not just the producers in the United States. And he really is probably the only person who can help them.”

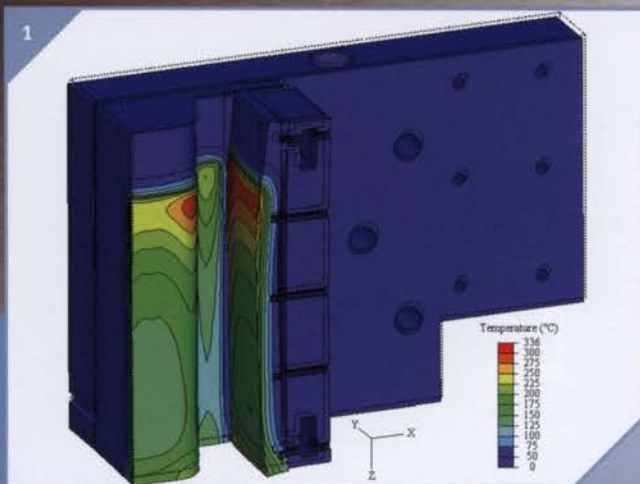
Another ongoing project is computational fluid-dynamics analysis of the turbulent flowing and solidifying steel to predict defects such as internal inclusions. The process includes using magnetic fields to manipulate the steel flow. This technique for controlling the flow of the molten steel also may improve its quality.

“Everyone knows if you properly apply magnetic fields then molten steel will change its flow direction, and may improve its quality,” says Thomas, “but it’s extremely difficult to do measurements of molten metal under magnetic fields to optimize this process—it’s a very harsh environment to physically venture into with sensors.”

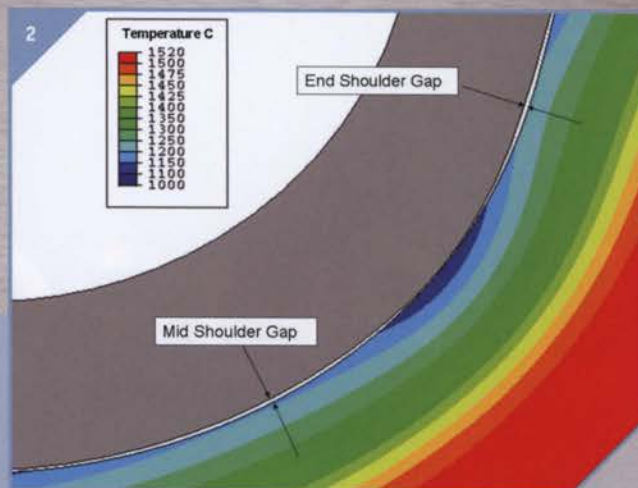
Casting steel with fewer defects makes safer steel products. Thomas says with the improved modeling methodologies, and the application results obtained with those models, his team has provided a better understanding of how defects such as internal inclusions and cracks form during the casting process (including the formation of breakouts) and improved the design of key casting variables, such as nozzle geometry and mold taper, which enable windows of casting parameters to produce steel with fewer defects.

The results obtained using supercomputers have been described in over 100 technical publications and have been implemented by the





1) 3D mold temperature results (distortion magnified 20x). A full 3D finite element model of one-fourth of the mold and water box was constructed to accurately calculate mold temperature and mold distortion. Much of the actual detail of the mold geometry was included in the model, such as the casting radius on the hot face, water channels and bolt holes.



2) Shoulder shell temperature contours with gap detail at 457 mm below meniscus.

member steel companies of the CCC. In addition, Thomas teaches short courses on the continuous casting process to industry. Koric was given an adjunct faculty affiliation with the Mechanical Science and Engineering Department in 2010 for his extensive research collaborations and HPC support for Thomas and other MechSE faculty members. Thomas also teaches about the continuous casting process and computational models in courses to his students.

Decreasing the material scrapped due to defects such as cracks, even by a small percentage, results in a large net savings to steel manufacturers and customers. Based on the roughly 100 million tons of steel produced each year in the United States and approximately \$400 per ton net cost of scrapping, a 1 percent reduction in yield loss would save about \$400 million per year. Increasing casting speed and decreasing spray cooling to conserve just 10 percent more of the internal energy of the strand would produce energy savings during reheating of \$350 million per year (based on \$0.06 per kilwatt hour) and an associated decrease in emissions.

"We want to find out ways to make the steel as safe and high quality as we can, and at the same time be very cost competitive," Thomas says. "My expertise is on the computational modeling side, but I want to make a real world impact." □

*Seid Koric and Brian Thomas were awarded the HPC Innovation Excellence Award for their work with CCC. (See page 27.)*

## PROJECT AT A GLANCE

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Brian Thomas  
Pratap Vanka

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### FUNDING

Continuous Casting Consortium members  
National Science Foundation

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<http://ccc.illinois.edu/>

### ACCESS ONLINE

[www.ncsa.illinois.edu/News/Stories/Steel](http://www.ncsa.illinois.edu/News/Stories/Steel)



By Trish Barker

Simulations using NCSA's Abe help psychologists

better understand how human beings

carve out cultural niches.

# DIFFERENT STROKES FOR DIFFERENT FOLKS



**HERE IS NO SUCH THING** as a person without culture," says University of Illinois psychology professor Dov Cohen. While we all have our individual characteristics and quirks, we're also

greatly influenced by the distinct ways of living, acting, and even thinking that surround us from the moment we're born.

For example, various experiments indicate that Western culture is generally more individualistic and analytical, while East Asian culture is more collectivist and holistic. In one often-cited experiment, members of both cultures were asked to describe what they saw in an aquarium. Westerners tended to single out the big fish in the foreground, while the Easterners were more likely to describe the scene as a whole.

Note the qualifications in that paragraph, however. "Generally." "Tended to." "More likely." Culture does not stamp out cookie-cutter people. There are always individuals who don't conform to the general trend.

"Usually, you consider that unexplained behavior 'error,'" says third-year graduate student Ivan Hernandez. "Which is like saying, we don't really know why it's going on, but let's kind of ignore it for now."

Cohen thought a computer model could help him better understand this intra-culture variability. Cohen, Hernandez, and Karl Dach-Gruschow, who earned his PhD in psychology from Illinois in spring 2010, used Northwestern's NetLogo modeling environment to develop an agent-based model of cultural evolution. Using the Abe supercomputer at NCSA, the team repeatedly ran their model,





generating multiple cultural outcomes and comparing them to what's known from observation and experiments. Their preliminary results were presented in 2010 at The Conference on Honor in Barcelona and have been accepted for a presentation at the 2012 conference of the Society for Personality and Social Psychology.

### Evolution in action

The model begins with a population of agents. Each one is defined by two characteristics—positive reciprocity (how likely is the agent to return a favor?) and negative reciprocity (how likely is the agent to pay back a wrong?).

High positive reciprocity and high negative reciprocity are characteristic of many “honor cultures,” often found among stateless people or in other environments where government can't be relied upon to provide support and right wrongs.

“They'll go through hell and high water to pay back a favor, and they pay back their debts, but they also make good on their threats,” Cohen says.

Other agents were a mix: high negative reciprocity and low positive reciprocity, low negative reciprocity and low positive reciprocity, etc.

The agents interact following simple rules. Agents that are high on negative reciprocity can command a certain amount of deference; but if two agents high on negative reciprocity meet and one is thought to have cheated the other, a feud can develop, resulting in a huge loss of resources for both parties. When any agent is depleted to zero resources, that agent disappears from the system. Agents that build

up a certain level of resources can reproduce, generating offspring who are likely to share their parent's characteristics.

“The computer simulations are incredibly useful, because they let you model evolution in action, the transmission of cultural ideas or ways of doing things from one generation to the next, from one adult to his or her successors,” Cohen says.

“It lets you examine how systems and the people within them develop,” Dach-Gruschow adds.

Each run of the model continues through hundreds of generations, and the model was run more than 1,200 times. That required more computer power than a simple laptop or even small cluster could provide.

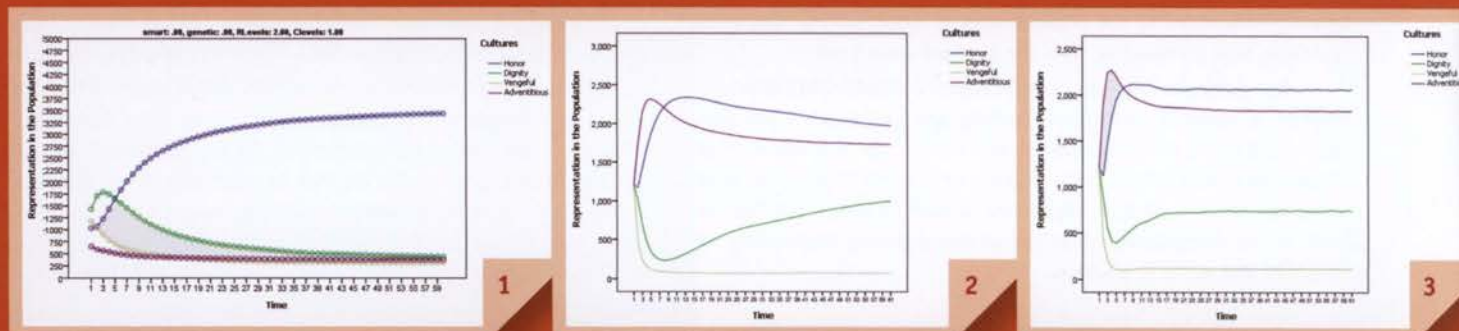
“It quickly became apparent that if you were going to do this seriously...you were going to need a lot of computing resources,” Cohen says. Celso Mendes, an Illinois computer scientist who frequently works with NCSA, recommended that Cohen apply for a start-up allocation on the center's supercomputers. “What they gave us really made this project possible, and every time we had a problem, it was a phone call away.

“NCSA has been so good to us. It's a great resource that's just tremendously helpful.”

### Room for difference

The culture generated by the interaction of agents in the model looked remarkably like the real world—a mix of different types of people.

“All of the types continue to exist, some at lower levels,” Cohen says. “In honor cultures, one of the most prevalent types are honor







people, but their exact opposite is also quite prevalent: People who in our model we call the 'adventitious'—they have no inclination to cooperate, they will minimally appease you if you absolutely make them, they will cheat if they can. But they also aren't punishers either. And we've found that in our lab experiments, too."

The results indicated that intra-culture variability is not error or noise, but instead that it's logical for individuals within a culture to follow a variety of strategies, some in step with the cultural norms and others diverging from them. Cohen, Hernandez, and Dach-Gruschow compare the results to the way animals carve out niches in their ecosystem. Among midshipman fish, for example, it's generally the largest males who win mates. But very tiny male midshipman fish are able to stealthily mate with female fish without being observed by their rivals. Both types of male can be successful.

"There is room, even when the predominant culture is one thing, to have people following a different cultural rule set," Hernandez says.

### Future research potential

As these preliminary results from their modeling efforts are presented at conferences, Cohen and Hernandez are gathering valuable feedback from their peers. They plan to continue to work with the model, trying different conditions and parameters. For example, would making the world of the model more settled lead to a less honor-based culture, which would support the current theory of how honor cultures evolve and devolve? What impact does a market economy have on culture? Law enforcement? Can the model illuminate the process through which one type of culture shifts to a different type of culture?

"It's hard to understand the origins of culture. We study the differences, but where do the differences come from originally?" Hernandez says. It's usually not possible to watch cultures evolve over many generations—unless the "people" are agents in a computer model. "This type of approach allows that to be possible." □

## PROJECT AT A GLANCE

### TEAM MEMBERS

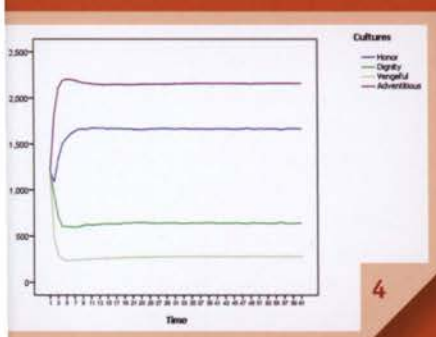
Dov Cohen  
Karl Dach-Gruschow  
Ivan Hernandez

### FOR MORE INFORMATION:

<http://www.psychology.illinois.edu/people/dovcohen>  
<http://ccl.northwestern.edu/netlogo/>

### ACCESS ONLINE

[www.ncsa.illinois.edu/News/Stories/difstrokes](http://www.ncsa.illinois.edu/News/Stories/difstrokes)



Charts from left to right: 1) Results of agent-based modeling where rewards for cooperation—and the risks of being taken advantage of—are relatively high. The Honor personality type (high positive reciprocity, high negative reciprocity) is the most successful strategy, though the other strategies continue to persist at lower levels. 2) Results of agent-based modeling under settings where rewards for cooperation—and the risks of being taken advantage of—are allowed to vary from low to high. The Honor personality type and its opposite, the Adventitious personality type (with low positive reciprocity, low negative reciprocity), are the most successful strategies. This graph represents a world with perfect transmission of strategy or personality type from parent to "offspring." 3) In this simulation, offspring were likely to resemble their "parent," but there was also some chance that offspring would choose the strategy that was most advantageous (regardless of the strategy of the parent). 4) In this simulation, offspring were likely to resemble their parent, but there was also some chance that offspring would either decide to pursue the strategy that is currently most advantageous or would simply pick a strategy at random. Above: Ivan Hernandez and Dov Cohen run models.





by Barbara Jewett

# BREAKING BUSINESS MODELS

**A**LMOST AS SOON AS NCSA OPENED, the center began collaborating with companies. One of the first was Eli Lilly. The firm used NCSA supercomputers to investigate leukotrienes, which cause the lungs to stiffen and become irritated. Investigators hoped to find a “receptor antagonist” that could block the leukotriene receptors without causing this reaction. By 1992, NCSA was helping Eli Lilly visualize the shapes of leukotriene molecules, moving from trial-and-error to rational drug design. That’s just one example of why a third of the FORTUNE 50 has worked with NCSA.

“What has made the NCSA Private Sector Program so successful for the past quarter-century,” explains Merle Giles, director of the NCSA Private Sector Program (PSP), “is that the program brings business and industry together with NCSA’s skilled staff and the best research minds at the University of Illinois.”

Through the years NCSA has worked with many multi-national companies—Boeing, Caterpillar, John Deere, Kodak, GE, Motorola, P&G, Rolls-Royce, Sears. Current partners (as of late 2011) are: ADM, Arbor Photonics, Boeing, BP, Caterpillar, John Deere, Dell, GE, IllinoisRocstar, Microsoft, Nimbis Services, Nokia Siemens Networks, P&G, Rolls-Royce, Waterborne Environmental, and John Zink.

In October 2011, PSP began offering partners a new compute cluster, iForge, which is dedicated to their use. It provides an end-to-end computing environment for PSP partners with an ability to handle pre- and post-data processing as well as simulations. It is especially well-suited for fluid dynamics and solid materials simulations.

## Research focus

While NCSA’s PSP team aids company researchers, the team also does some of their own research. They try to anticipate what partners will need to stay competitive so they can offer additional services or respond nimbly to requests. Currently the PSP team is excited to be involved in two research projects that will aid their industrial partners.

With a \$200,000 Early Concept Grant for Exploratory Research (EAGER) award from the National Science Foundation, PSP is documenting the use of science by the industrial computational community. They expect to aid understanding of the interplay between federally supported university-based research and industrial research and development, highlighting how interdependent academic and industrial science are. In addition, they hope to link to activities at a number of federal agencies and departments.

Industry demand for simulation-based engineering and science has increased due to a variety of factors, explains Giles. Companies face economic pressure to decrease time to market. They also need to utilize multi-disciplinary physics to address product complexity and safety, due to a general inability to conduct physical prototyping due to miniaturization, complex materials manipulation, or safety. Companies want to take advantage of modern production methods and energy innovation and conservation.

“Most HPC surveys focus on utilization of hardware, which is often expressed in terms of scale, such as the numbers of processor cores used simultaneously in a simulation,” says Giles. “We have observed that there are science and engineering limitations to the use of software, as

sophisticated as such software often is, and that these limitations are not well understood, and certainly not well documented.”

NCSA’s PSP is also a key service provider for the National Digital Engineering and Manufacturing Consortium (NDEMC), a U.S. public-private partnership tasked to demonstrate advancements in digital engineering and manufacturing through a \$5 million Midwest pilot project. The project has the attention and involvement of a U.S. agency not previously involved with HPC: the Department of Commerce. Current shareholders in the consortium include John Deere, General Electric, Lockheed Martin, the Department of Commerce’s Economic Development Administration, and the state of Ohio.

Working with the Ohio Supercomputer Center, the National Center



Merle Giles

for Manufacturing Sciences, and the Council on Competitiveness, the pilot project will, among other things, develop user-friendly web portals, lowering technical barriers to the utilization of sophisticated software applications. Small and medium manufacturing enterprises can then develop advanced computer modeling and simulation skills. NCSA will provide trainers and domain experts to select project companies.

## The next 25 years

When it comes to PSP, Giles continually looks forward. Data-intensive computing, data-driven computing, and computational data analytics are exciting fields that benefit from the sort of large-system expertise found among the Illinois’ campus faculty and the NCSA staff. PSP is currently working with several data projects and is in discussions on additional ones. Companies are drowning in data, he notes, and “managing that data is imperative so that companies can make intelligent decisions based on accurate, up-to-date information.”

“NCSA and PSP have significantly impacted how many major corporations conduct their business,” says Giles. “We’ve broken the standard business model for many of our partners.”

And as NCSA and PSP assist companies in leveraging end-to-end-digital solutions, they become competitive in an ever-changing global business climate. And that’s a business model everyone can appreciate.





# USER REFLECTIONS

**AL VALOCCHI**

*University of Illinois at Urbana-Champaign*

**Q. What were you studying when you used NCSA's first supercomputer, the Cray X-MP? What new results came from its use? What other NCSA capabilities helped you advance your science?**

Preparations for observing NCSA's 25th anniversary year in 2011 revealed several users who computed at NCSA in 1986 who are still active users today. We invited them to share their thoughts on advances in high-performance computing.

A. My general field of study is the same now as it was 25 years ago—numerical simulation of fluid flow and contaminant transport in the subsurface. Advanced scientific computing allows us to consider more complex and more realistic systems—for example, we can study mixtures of contaminants that participate in chemical and biological reactions and we can consider more complex geology. With the Cray X-MP, we were investigating transport of a single contaminant that was reacting with the soil for flow through a “layer-cake” geological system. Back then, this represented the leading edge of complexity.

Using the Cray X-MP allowed us to solve larger problems on finer grids. The numerical results revealed some emergent patterns at large time, and this led to development of new analytical mathematical results for predicting this large-time behavior.

**Q. In what ways has access to supercomputers at NCSA advanced your science since then?**

A. In general, access to supercomputers (at NCSA and elsewhere) has permitted study of more complex and realistic problems. As we learn more about the geology, physics, chemistry, and microbiology of the sub-surface, we develop more rigorous and sophisticated mathematical models. Numerical solution of

these models is a computational “grand challenge” that requires supercomputers. Also, due to the inherent uncertainty about subsurface geology, we need to simulate flow and transport over and over multiple times in different alternative and equally likely models of the subsurface geology.

**Q. In what areas do you envision advances in supercomputing capability having the most impact in your research during the coming 5-10 years?**

A. There will be advances on two fronts. First, as mentioned already, we will consider more complex physical problems. As an example, consider the greenhouse gas mitigation strategy known as “carbon capture and storage,” in which supercritical carbon dioxide is injected into deep saline aquifers. (In fact, the Illinois State Geological Survey is about to start a unique pilot demonstration project at the ADM facility in Decatur.) In order to study the feasibility and long-term safety, we need sophisticated three-dimensional models that include multiple fluid phases, density, temperature and geomechanical effects, many different chemical reactions; moreover the models must consider very large spatial domains (hundreds of kilometers) and long time scales (thousands of years). This is a very challenging computational problem.

The second area of advancement connected to supercomputing will be new methods for uncertainty quantification and parameter estimation. Due to the difficulty of sampling and observing the subsurface, stochastic models are preferred to deterministic models. There have been some new Bayesian methods proposed that seek to find the entire probability distribution of the key quantities, but these methods are computationally expensive.

**Q. Is there anything supercomputers enabled you to do 20-25 years ago that you thought was really “wow” and cutting-edge at the time, but that you look back at now and smile at the memory of how “high tech” you thought you were at the time?**

A. I can remember doing some 2D visualizations of our simulations. We were proud of those visualizations, but looking back they were primitive compared to the software and hardware tools available today at a fraction of the cost.



by Diana Yates

# LEAP TO WHOLE-CELL SIMULATIONS

**R**ESearchers have built a computer model of the crowded interior of a bacterial cell that—in a test of its response to sugar in its environment—accurately simulates the behavior of living cells.

The new “*in silico* cells” are the result of a collaboration between experimental scientists at the Max Planck Institute of Biology in Germany and theoretical scientists at the University of Illinois using the newest graphics processing unit (GPU) computing technology on NCSA’s now-retired Lincoln cluster as well as a GPU cluster that is part of Illinois’ CUDA Center of Excellence.

Their study appears in the journal *PLoS Computational Biology*.

“This is the first time that we’re modeling entire cells with the complete contents of the cellular cytoplasm represented,” says Illinois postdoctoral researcher and lead author Elijah Roberts. “We’re looking at the influence of the whole cellular architecture instead of modeling just a portion of the cell, as people have done previously.”

University of Illinois chemistry professor Zaida Luthey-Schulten, who led the research, had done molecular dynamics simulations of individual molecules or groups of molecules involved in information processing, but never of a system as large and complex as the interior of an entire cell.

Then in 2006 she saw a paper by Wolfgang Baumeister and his colleagues at Max Planck that located every one of a bacterium’s ribosomes, its protein-building machines, inside the cell.

That image spurred Luthey-Schulten to think about modeling an entire cell, and she asked Baumeister and his colleague Julio Ortiz if they would repeat the study in *Escherichia coli* (*E. coli*), a bacterium that has been the subject of numerous molecular studies.

Once the new ribosome data were available, Roberts looked to other studies that described the size distribution of the rest of the molecules that take up space in the cell. By adding these to the ribosome data, he developed a three-dimensional model that showed the degree of “molecular crowding” in a typical *E. coli* cell.

Luthey-Schulten was amazed at how little “space” remained inside the cell, she says.

“I think, like everybody else, my perception of the cell up until Wolfgang and Julio’s 2006 article had always been that it’s a pretty big sack of water where a lot of chemical reactions occur,” she says.

“But in fact there are a lot of obstacles in the cell, and that is going to affect how individual molecules move around and it’s going to affect the reactions that occur.”

Other researchers have begun studying the effects of molecular crowding on cellular processes, but never at the scale of an entire cell.

Those studying live cells can—by conducting fluorescence experiments—discover variations in the copy number of a particular protein in a population of cells. But they are less able to observe the microscopic details that give rise to such differences between genetically identical cells. Well-designed computer simulations of whole cells can track every reaction within the cells while also accounting for the influence of molecular crowding and other variations between cells, Luthey-Schulten says.

For example, by running simulations on models of two *E. coli* strains, the researchers were able to see that “bacterial cell architecture does indeed affect the reactions that occur within the cells,” Luthey-Schulten says. When sugar was present in its environment, a longer, narrower *E. coli* strain was able to ramp up production of a sugar-transporter protein much more quickly than a bigger strain, the researchers found. That difference had a lot to do with the distribution of molecules in each cell type, Roberts says.

The computer simulation also showed how molecular crowding influences the behavior of a molecule that, when it binds to DNA, shuts down production of the sugar-transporter protein. Even when it wasn’t bound to DNA, this repressor remained close to the binding site because other molecules in the cell blocked its escape. These intracellular obstacles reduced its ability to diffuse away.

The new model is only a first step toward an accurate simulation of a whole working cell, the researchers say. The development of better models will rely on the work of those conducting research on actual cells. Their data provide the framework for improving computer models, Luthey-Schulten says, and offer a real-world test of the “*in silico* cells” ability to recreate the behavior of living cells.

Future studies will further develop the *E. coli* models and will focus on methane-generating archaeal microbes.

Diana Yates is the life sciences editor for the University of Illinois News Bureau. ■



## NCSA ADDS SYSTEMS, RETIRES OTHERS



Forge—a 153-teraflop supercomputer that combines both CPUs and general-purpose graphics-processing units (GPUs)—is now available at NCSA for use by scientists and engineers across the country. Multiple scientific codes have been adapted for GPU computing, enabling a rapidly diversifying range of research, including biomolecular simulations, lattice quantum chromodynamics, computational fluid dynamics, cryptography, and molecular dynamics.

Seventy percent of the compute time Forge offers will be allocated through the National Science Foundation's Extreme Science and Engineering Discovery Environment (XSEDE) program. XSEDE, a cross-country partnership of nearly 20 institutions, is led by NCSA and provides digital resources, services, tools, and support to the nation's science and engineering research community. The remaining 30 percent of Forge's cycles will be allocated to NCSA's Private Sector Program and to faculty, staff, and students at the University of Illinois at Urbana-Champaign.

Forge joins an SGI system called Ember at the University of Illinois' National Petascale Computing Facility. Ember, which previously was allocated through the NSF's now-concluded TeraGrid program, will now be used by Illinois faculty, staff, and students, by NCSA's private sector partners, and by other researchers at the discretion of NCSA's leaders.

Forge combines 18 Dell PowerEdge C6145s that contain 36 nodes of dual-socket/eight-core AMD processors with M2070 NVIDIA Fermi GPU units housed in Dell's C410x PCI expansion enclosures. There are eight Fermi units for each node, for a total of 288. Each NVIDIA M2070 provides more than 500 gigaflops of double-precision performance and 6GB of GDDR5 memory. Forge also has a QDR InfiniBand interconnect, 700 terabytes of GPFS filesystem space provided by two Data Direct Networks SFA 10000 units, and an I/O bandwidth that exceeds 16GB/sec.

Lincoln, the center's previous GPU-CPU system, is now retired. Earlier this year, the center also retired the Abe supercomputer.

## NCSA LEADS PROJECT ON SCIENCE GATEWAY SECURITY

A three-year project to improve security for science gateways used by researchers across the country is under way, led by NCSA in collaboration with Indiana University, the Texas Advanced Computing Center (TACC), and the University of Wisconsin-Madison.

The "Distributed Web Security for Science Gateways" project, which is supported by a \$948,821 grant from the National Science Foundation's Software Development for Cyberinfrastructure program, will enhance cyberinfrastructure for research and education by providing common software building blocks for science gateway security. These building blocks will facilitate secure connections between science gateways and other cyberinfrastructure, increasing the trust in science gateways by scientists and resource providers.

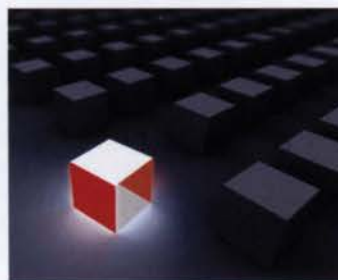
Jim Basney, an NCSA senior research scientist, is the project's principal investigator. Co-PIs are Marlon Pierce of Indiana University and Rion Dooley of TACC.

Science gateways broaden and simplify access to cyberinfrastructure by providing web-based interfaces to collaboration, analysis, data management, and other tools for students and researchers. The new project will provide authorization and delegation software for science gateways that complies with the standard OAuth protocol, which has been widely adopted in the Web 2.0, cloud, and social networking worlds. The project will also build on and integrate with the Open Gateway Computing Environments (OGCE) platform.

The project is partnering with three scientific research projects: UltraScan, iPlant, and GridChem, and with the Middleware Security and Testing (MIST) team for independent security evaluation of the software to be developed.

For more information about the project, please visit [www.sciencegatewaysecurity.org](http://www.sciencegatewaysecurity.org).

## ILLINOIS LAUNCHES PARALLEL COMPUTING INSTITUTE



The University of Illinois' Coordinated Science Laboratory has launched a new interdisciplinary institute to provide the resources to enable breakthroughs in parallel computing.

The Parallel Computing Institute, led by computer science professor William Gropp, who is also NCSA's deputy director for research, draws upon the university's strength in parallel



computing to arm researchers and educators with the support they need to address major computational challenges in science, engineering, health and business, among other areas.

PCI will serve as an incubator for developing and sustaining interdisciplinary centers and initiatives in parallel computing by expanding access to resources and infrastructure, teaching critical skills to graduate and undergraduate students, creating more opportunities for funding, establishing key external partnerships, and sharing expertise with research teams who want to do high-impact work in parallel computing.

Today's programmers often lack the skills necessary to write code for many-core systems. One of PCI's early thrusts will be research and education that make it easier to program on parallel platforms. An example of such research includes the development of middleware that translates the CUDA programming language for field-programmable gate arrays, an adaptable, low-power chip solution.

More information is available at  
[www.csl.uiuc.edu/institutes/parallel-computing-institute](http://www.csl.uiuc.edu/institutes/parallel-computing-institute).

## SNIR CHOSEN TO LEAD DIVISION OF ARGONNE



Illinois computer science professor and Blue Waters co-principal investigator Marc Snir has been chosen to direct the Mathematics and Computer Science Division (MCS) at Argonne National Laboratory (ANL). Snir has been a leader in shaping high performance computing (HPC) architectures and parallel programming, including contributions to IBM's

SP and Blue Gene systems and to MPI, the standard communications library used in HPC. At MCS, he will be directing over 200 researchers and staff members who are working on projects ranging from algorithm development and software design in key areas like optimization, to exploration of new technologies such as distributed computing and bioinformatics, to numerical simulations in challenging areas like climate modeling. Snir will continue to hold his appointment as professor of computer science. He will divide his time between MCS and the University of Illinois and will continue to be associated with the Blue Waters project.

A distinguished researcher and scholar, Snir chaired the Department of Computer Science at the University of Illinois Urbana-Champaign from 2001 to 2007. While at Illinois, he also co-directed the Intel and Microsoft Universal Parallel Computing Research Center, was the first director of the Illinois Informatics Institute, and is the associate director for extreme-scale computing at NCSA. In addition, Snir co-chaired the National Research Council's Committee to Study the Future

of Supercomputing, and he is a co-author of its influential 2004 report, "Getting Up to Speed: The Future of Supercomputing."

## NCSA DIRECTOR DUNNING ELECTED ACS FELLOW



Thom Dunning directs NCSA and also holds the Distinguished Chair for Research Excellence in Chemistry at the University of Illinois. He is one of four Illinois chemistry professors among 213 distinguished scientists elected fellows of the American Chemical Society this year. The others are Catherine Murphy, Ralph Nuzzo and Jonathan Sweedler. Dunning's research

focuses on the development of techniques for the accurate solution of the electronic Schrödinger equation, and on new computational approaches to enhance scientists' understanding of, and ability to predict, the structure, energetics and reactivity of molecules.

## NCSA AWARDED \$7.7 MILLION FOR DES DATA MANAGEMENT

The National Science Foundation has awarded a grant of \$7.7 million over five years to NCSA to operate a sophisticated data management pipeline for the Dark Energy Survey, a collaborative astronomy project focusing on uncovering the nature of dark energy.

Beginning in 2012, the DES will use a 500-megapixel camera (DECam) to deeply image 10 percent of the sky for 500 nights, producing a precise picture of the largest-scale structures in the universe and a detailed measurement of how those structures have evolved over time. DES will gather an enormous amount of data, capturing terabytes every night.

"This type of data-intensive, data-driven science requires networking, computing, and archiving capabilities and sophisticated tools to efficiently process the data," says Don Petravick, who leads the DES data management project. "It's our role at NCSA to provide those capabilities and tools as an integral part of the DES collaboration. This allows astronomers to focus on analysis of science-ready data, rather than spending their time on preliminary processing or technical issues."

Working closely with the DES collaboration and the Illinois Department of Astronomy, NCSA has developed a system for processing, calibrating, and archiving the wealth of data that will be gathered by the DES. This system will use high-performance computing resources provided by the NSF's XSEDE (Extreme Science and Engineering Discovery Environment) project.



## News &amp; Notes

NCSA and the University of Illinois have been involved in the DES collaboration since 2005. The data management tools have been tested through periodic Data Challenges, working with simulated data that has progressively become closer and closer in volume and complexity to what will be gathered when DES comes online next year.

NCSA is also involved in the data management system for the upcoming Large Synoptic Survey Telescope (LSST), which will use an 8.4 meter telescope and 3 gigapixel camera to produce a wide-field astronomical survey of the universe that tracks its changes over time. Like DES, LSST will collect terabytes of data every night.

"We'll process the images of 30 million stars and galaxies for each full night of observing," Petravick says.

For more information, go to: <http://cosmology.illinois.edu/DES/>.

## VISUALIZATION TEAM AIDS ORIGINAL MOVIE



Members of the Illinois Emerging Digital Research and Education in Arts Media Institute (eDream) and the Advanced Visualization Laboratory (AVL) at NCSA created data-driven visualizations of the Mississippi River Valley showing the extent of destructive 1927 floodwaters for the 75-minute multimedia work "The Great Flood." The work features Grammy Award-winning guitarist and composer Bill Frisell performing original music with accompanying film and staging by Obie-winning experimental filmmaker Bill Morrison. It premiered in September 2011 at the University of Illinois.

In the spring of 1927, the Mississippi River surged over its banks in 145 places after 15-inch downpours followed the heavy rains of the previous summer. Levees across the Midwest and the plains failed, and the surging water inundated 27,000 square miles to a depth of up to 30 feet. Part of

the flood's enduring legacy was the mass exodus of displaced sharecroppers thereby ensuing transformation of American society and music.

The eDream/AVL team drew on a 1920s map of the river and contemporary geospatial data to visualize a journey along the Mississippi, providing context for documentary footage from the era. eDream and AVL contributors to the project were Donna Cox, director of eDream and AVL, research artist Robert Patterson, research programmers Alex Betts and Stuart Levy, and media specialist Jeff Carpenter.

University of Illinois geography professor Shaowen Wang, who also leads NCSA's efforts in advanced geographic information systems, and members of his research team—research scientist Yan Liu, visiting scholar Kai Cao, and students Su Han and Yanli Zhao—helped access and process the GIS data, which was scattered across multiple government websites and databases. The geography team also helped to assign coordinates to the historical map so the contemporary data could be aligned to it. AVL's Betts developed custom plug-in capabilities for the Maya animation software to enable integration and visualization of large geospatial datasets, including high-resolution elevation data, land use data and the historical flood data. This will provide capabilities for future GIS visualization projects.

## KORIC, THOMAS, RECEIVE IDC INNOVATION AWARD



Brian Thomas



Seid Koric

Helped by NCSA, the Continuous Casting Consortium (CCC) at the University of Illinois has developed comprehensive numerical models of the continuous casting of steel, including several ground-breaking numerical methods, to solve practical problems of interest to the steel industry. (See the article on page 16.)

The CCC is directed by mechanical science and engineering professor Brian Thomas with NCSA's Seid Koric. Their work with CCC earned them the HPC Innovation Excellence Award from International Data Corporation in November 2011.

The award distinguishes noteworthy achievements made by projects that make significant use of HPC. Recipients are those who have successfully applied HPC to improve business, scientific advancement, and/or engineering successes.



# BIOGEE





# R ISN'T BETTER

**F**OR SOME COMPLEX BIOLOGICAL STRUCTURES, bigger isn't always better. Instead what most researchers want to explore is the actions of smaller biological structures over longer periods of time.

Researchers from the University of Utah, University of California at San Diego, Rutgers University, Stony Brook University, and the University of Florida have teamed up to get a closer—and longer—look at those smaller proteins through the National Science Foundation's Petascale Computing Resource Allocations (PRAC) program. The PRAC program supports science teams as they work with NCSA to run on Blue Waters and other petascale systems.

Molecular dynamics research captures the interactions of individual atoms in complex biological structures like proteins, DNA, and RNA. Looking at smaller systems of atoms isn't necessarily easier than looking at ever-larger systems, explain the researchers, because molecular dynamics is very difficult to parallelize as you can't parallelize for time.

A researcher wrings performance out of today's supercomputers by breaking a problem up into many small pieces and having those pieces run simultaneously on the computer's many processors. Because the atoms in the simulation are influenced by what has happened at previous points in the simulation, you can't have the future proteins or RNA being simulated at the same time as their earlier selves. You have to take it one timestep at a time.

So the team is looking at a process where you have lots of simulations, but the processors share moderate amounts of information that are really crucial to solving the overall problem.

Using this intermediary approach, the team runs multiple copies of the same system under different conditions, simulating the system at a variety of high temperatures, pH levels, or even physics models not typically found in nature, for example. These copies swap data every so many timesteps within the calculation.

Scientists have been using this method—called replica exchange—for about a quarter of a century. However, with recent access to large-scale HPC resources through the TeraGrid and XSEDE, the use of these methods has exploded. In fact, the team and others have seen a series of successes by using it. On Blue Waters and other systems of its size, the team wants to begin enabling multidimensional replica and information exchange between ensembles of independent molecular dynamics simulations, delving into the effects of changes to more than one factor that influence the system's behavior. They've learned that only looking at one factor isn't enough.

As part of the PRAC program the team is currently updating the simulation code frequently used to do that work. Called AMBER, more than 1,000 sites around the world take advantage of the code.

*Shown here: DNA interstrand crosslinks (ICLs) are formed by agents with the ability to covalently link two strands of duplex DNA. ICLs are extremely cytotoxic, since they block essential processes such as DNA replication and transcription. ICL-inducing agents such as cisplatin are widely used in cancer chemotherapy. Simulations are being used to gain insight into the effect of ICLs on DNA, and mechanisms by which tumor cells can become resistant to treatment. □*





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